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14. ABSTRACT

We describe enhancements under development for multi-scale methods to be applied to the high-fidelity modeling of spacecraft electric propulsion systems and their environment. Multiple challenges in multi-scale integration, statistical accuracy, and physical modeling are addressed through a variety of innovative numerical methods and mathematical approaches. We emphasize the advances made on a specialized multi-scale time-stepping integrator for finite-Larmor radius particle trajectories, accelerated collisional-radiative non-equilibrium ionization kinetics through Boltzmann equilibrated level groups, and a novel approach to dynamic phase-space reconstruction which can be used to resolve the problems of multi-scale statistics in particle-based kinetic simulations.

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ACCELERATION OF PIC AND CR ALGORITHMS FOR HIGH FIDELITY IN-SPACE PROPULSION MODELING

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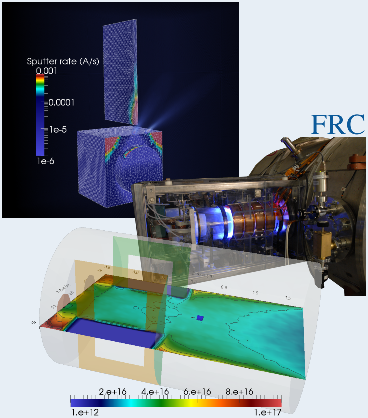
OUTLINE

Spacecraft Propulsion Relevant Plasma:

- From hall thrusters to plumes and fluxes on components
- Complex reaction physics i.e. Discharge and Breakdown in FRC
- Relevant Densities often Span 6+ Orders of Magnitude
- Spatial scales of interest span μm-100m range

Electric Propulsion Plumes



Chamber Environment

Spacecraft Plasma Modeling Challenges

Spacecraft Propulsion Relevant Plasma:

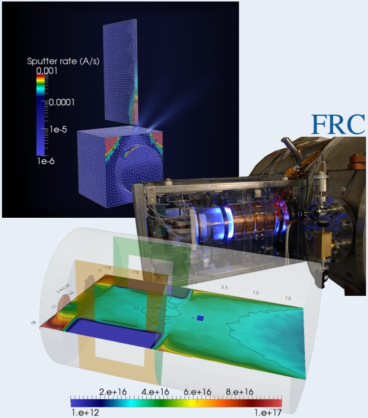
- From hall thrusters to plumes and fluxes on components
- Complex reaction physics i.e. Discharge and Breakdown in FRC
- Relevant Densities often Span 6+ Orders of Magnitude
- Spatial scales of interest span μm-$100 m$ range

Solution?

Multi-Scale and Multi-Physics Adaptive Algorithms

Electric Propulsion Plumes

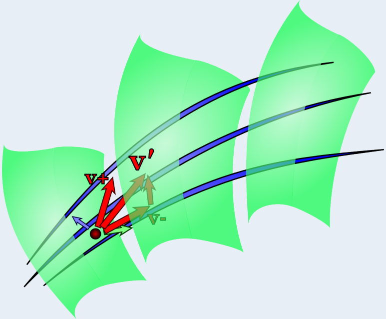
FRC



Chamber Environment

Boris Push:

$$
\begin{aligned}
v^- &= v(t-\Delta t/2) + \frac{q\Delta t}{2m}E(t) \\
v' &= v^- + \frac{q\Delta t}{2m}v^- \times B(t) \\
v^+ &= v^- + \frac{\frac{q\Delta t}{2m}}{1+\left(\frac{q\Delta t}{2m}|B|\right)}v' \times B(t) \\
v(t+\Delta t/2) &= v^+ + \frac{q\Delta t}{2m}E(t) \\
r(t+\Delta t) &= r(t) + \Delta t v(t+\Delta t/2)
\end{aligned}
$$



MULTI-SCALE PARTICLE ADVANCEMENT

Boris Push:

$$
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v(t{+}\Delta t/2) &= v^+ + \frac{q\Delta t}{2m} E(t) \\
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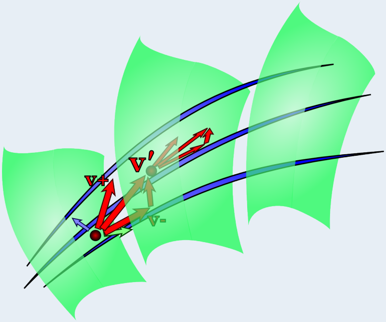
- Leap-Frog in r & v



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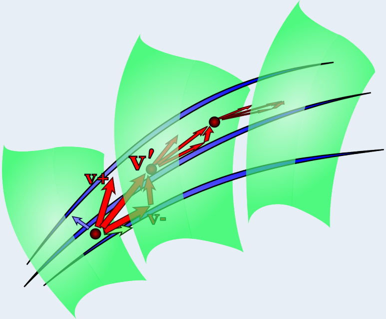
- Leap-Frog in r & v
- Energy Conservation only via Interpolation in Time



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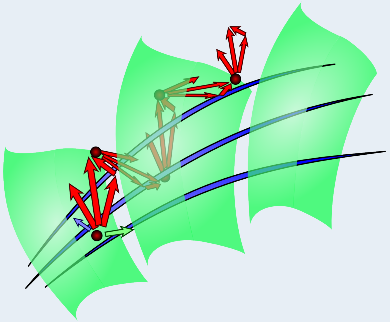
- Leap-Frog in r & v
- Energy Conservation only via Interpolation in Time
- Numerically Stable but Drifts and Fails when $\Delta t > \omega_c/2$



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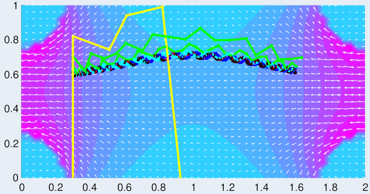
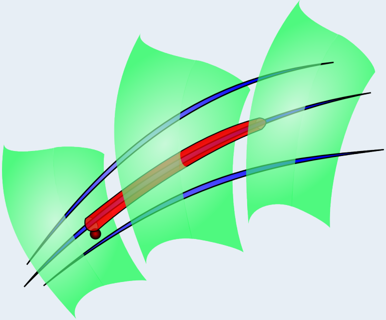


Magnetic Mirror Test

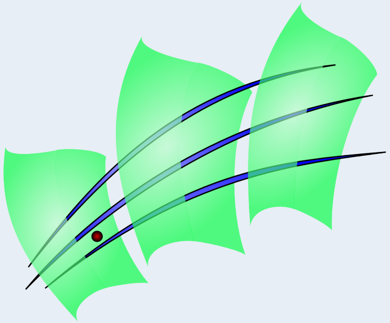
Gyrokinetic Push:

- Effective for High-B Plasma (i.e. Magnetic-Fusion)
- Assumes $\lambda_c \ll dx$
- Looses Phase Information
- Assumes Phase-Scatter Diffusion Negligible



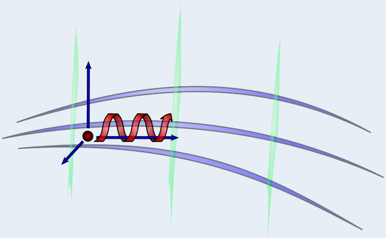
B-Frame Push:

- Coordinates Rotated and Aligned to *B*-Field



B-Frame Push:

- Coordinates Rotated and Aligned to B-Field
- Motion Decomposed into Rotation and Drift
- Exact Solution in Constant Field



B-Frame Push:

- Coordinates Rotated and Aligned to B-Field
- Motion Decomposed into Rotation and Drift
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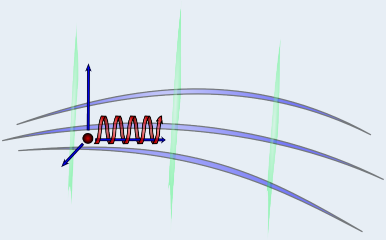
- Phase Preserved Across Many-ω_c



B-Frame Push:

- Coordinates Rotated and Aligned to B-Field
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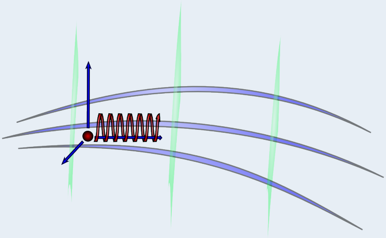
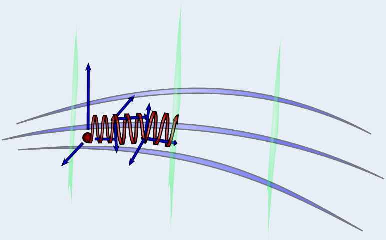
What about Variable Fields?



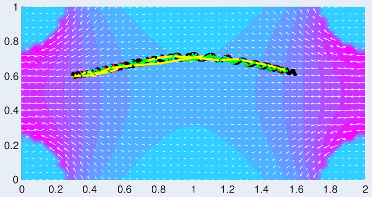
B-Frame Push in Variable Fields:

- Consistent Solution Recovered with Multiple Steps



B-Frame Push in Variable Fields:

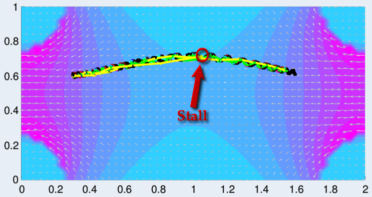
- Consistent Solution Recovered with Multiple Steps
- Convergence Order is Low



Magnetic Mirror Test

B-Frame Push in Variable Fields:

- Consistent Solution Recovered with Multiple Steps
- Convergence Order is Low
- Solution Stalls when $dt > \omega_c$



Magnetic Mirror Test

B-Frame Push in Variable Fields:

- Consistent Solution Recovered with Multiple Steps
- Convergence Order is Low
- Solution Stalls when $dt > \omega_c$
- Consider the Push in $\hat{B}$-Aligned Coordinates...
- No Mechanism for $v_\perp \rightarrow v_\parallel$ in Step?
  (No Bounce in Magnetic Mirror?)
- Variable $\vec{B}$ and $\vec{E}$ via Taylor Series?

$$\Delta\vec{v} = \mathbf{D}_0 \cdot \vec{v} + \frac{q\Delta t}{m}\mathbf{D}_1 \cdot \vec{E}$$

$$\Delta\vec{x} = \mathbf{D}_1 \cdot \vec{v}\Delta t + \frac{q\Delta t^2}{m}\mathbf{D}_2 \cdot \vec{E}$$

$$\mathbf{D}_k = \hat{\mathbf{R}}^{-1} \cdot \Delta_k \cdot \hat{\mathbf{R}}$$

$$\Delta\mathbf{v}^R = \underbrace{\begin{pmatrix} -C_0 & S_0 & 0 \\ -S_0 & C_0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\Delta_0} \cdot \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} + \underbrace{\begin{pmatrix} S_1 & C_1 & 0 \\ -C_1 & S_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\Delta_1} \cdot \begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix}$$

$$\Delta\mathbf{x}^R = \underbrace{\begin{pmatrix} S_1 & C_1 & 0 \\ -C_1 & S_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\Delta_1} \cdot \begin{bmatrix} v_x\Delta t \\ v_y\Delta t \\ v_z\Delta t \end{bmatrix} + \underbrace{\begin{pmatrix} C_2 & -S_2 & 0 \\ S_2 & C_2 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}}_{\Delta_2} \cdot \begin{bmatrix} a_x\Delta t^2 \\ a_y\Delta t^2 \\ a_z\Delta t^2 \end{bmatrix}$$

B-Frame Push in Variable Fields:

- Consistent Solution Recovered with Multiple Steps
- Convergence Order is Low
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- No Mechanism for $v_\perp \to v_\parallel$ in Step?
  (No Bounce in Magnetic Mirror?)
- Variable $\vec{B}$ and $\vec{E}$ via Taylor Series?

But even $\hat{R}$ depends on $\vec{B}$
(And is Partially Arbitrary!)

$$\Delta\vec{v} = \mathbf{D}_0 \cdot \vec{v} + \frac{q\Delta t}{m}\mathbf{D}_1 \cdot \vec{E}$$

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B-Frame Push in Variable Fields (cont.):

- Push as Explicit Matrix Operator:
  (For now Ignoring $\vec{E}$)

$$\mathbb{X}_+ = \mathbb{M} \cdot \mathbb{X}_0$$

$$\mathbb{X}_+ = \begin{bmatrix} \vec{x}_+ \\ \vec{v}_+ \end{bmatrix} = \begin{bmatrix} \vec{x_0} + \Delta\vec{x} \\ \vec{v_0} + \Delta\vec{v} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbb{I} & \mathbf{D}_1 \\ 0 & \mathbb{I} + \Delta t \mathbf{D}_0 \end{bmatrix}}_{\mathbb{M}} \cdot \begin{bmatrix} \vec{x}_0 \\ \vec{v}_0 \end{bmatrix}$$

B-Frame Push in Variable Fields (cont.):

- Push as Explicit Matrix Operator:
  (For now Ignoring $\vec{E}$)
- What's Known about $\mathbb{M}$:
  - Reversible through Time Inversion...
  - $\mathbb{M}^{-1}$ Must Exist
  - $\mathbb{M}$ is a 1:1 Map of $\mathbb{X}_0 \rightarrow \mathbb{X}_+$
  - $\mathbb{M}$ is Unique (Even if $\hat{R}$ was Not...)
  - If $\mathbb{M}$ is Unique, Elements are Unique
  - $\mathbb{M}$ is Constant if $\vec{B}$ is Constant

$$\mathbb{X}_+ = \mathbb{M} \cdot \mathbb{X}_0$$

$$\mathbb{X}_+ = \begin{bmatrix} \vec{x}_+ \\ \vec{v}_+ \end{bmatrix} = \begin{bmatrix} \vec{x_0} + \Delta\vec{x} \\ \vec{v_0} + \Delta\vec{v} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbb{I} & \mathbf{D}_1 \\ 0 & \mathbb{I} + \Delta t \mathbf{D}_0 \end{bmatrix}}_{\mathbb{M}} \cdot \begin{bmatrix} \vec{x}_0 \\ \vec{v}_0 \end{bmatrix}$$

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Hypothesis:

Elements of $\mathbb{M}$ Vary Smoothly, $\vec{x} \underset{\text{Ngbh}}{\in} \vec{x}_0$

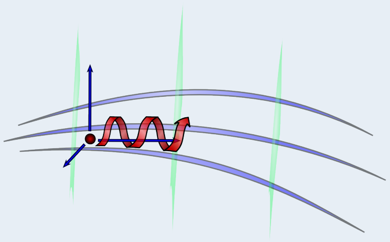
(Assuming $\vec{B}$ Varies Smoothly with $\vec{x}$)

$$\mathbb{X}_+ = \mathbb{M} \cdot \mathbb{X}_0$$

$$\mathbb{X}_+ = \begin{bmatrix} \vec{x}_+ \\ \vec{v}_+ \end{bmatrix} = \begin{bmatrix} \vec{x_0} + \Delta\vec{x} \\ \vec{v_0} + \Delta\vec{v} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbb{I} & \mathbf{D}_1 \\ 0 & \mathbb{I} + \Delta t \mathbf{D}_0 \end{bmatrix}}_{\mathbb{M}} \cdot \begin{bmatrix} \vec{x}_0 \\ \vec{v}_0 \end{bmatrix}$$

B-Frame Push in Variable Fields (cont.):

- Assuming $\vec{B}$ varies Periodically in ω_c and Linearly in multiples $N \times \omega_c$...?



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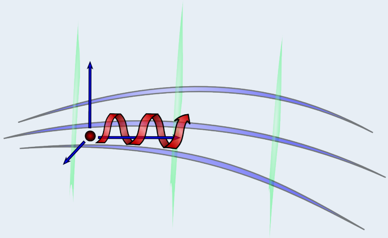
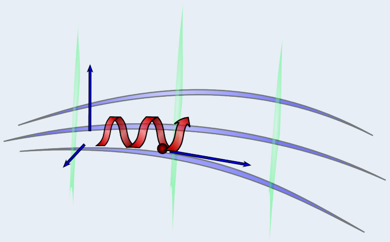


B-Frame Push in Variable Fields (cont.):

- Assuming $\vec{B}$ varies Periodically in ω_c and Linearly in multiples $N \times \omega_c$...?
- Elements of $\mathbb{M}$ take Form:

$$m_{ij} = \overline{m}_{ij} + \frac{n\delta t}{\Delta t}\Delta m_{ij}^{[slow]} + cos(\omega n\delta t)\Delta m_{ij}^{[c]} + sin(\omega n\delta t)\Delta m_{ij}^{[s]}$$



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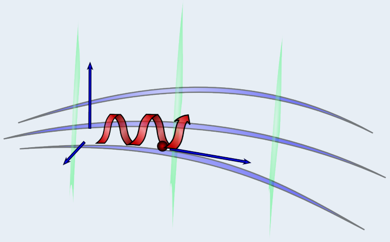
- Coefficients, Δm_{ij}, can be Sampled using Original Push with $\Delta t = [0, \pi/4, 3\pi/4, 2\pi n]\omega_c$



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- Assuming $\vec{B}$ varies Periodically in ω_c and Linearly in multiples $N \times \omega_c$...?
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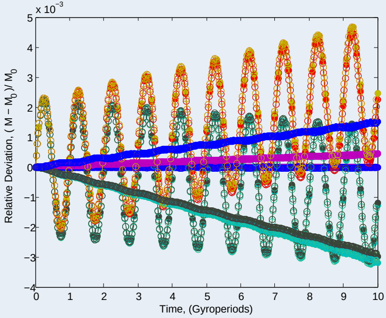
- Coefficients, Δm_{ij}, can be Sampled using Original Push with $\Delta t = [0, \pi/4, 3\pi/4, 2\pi n]\omega_c$
- Comparison of Fit and Sampled $\mathbb{M}$ from Magnetic Mirror



Closed Circle - Original Push Stepping m_{ij}
Open Circle - Estimated m_{ij} from Sampling

Compounded Push Operator:

- Uniform Field Push can be Subdivided

Compounded Push Operator:

- Uniform Field Push can be Subdivided

$$\mathbb{X}(t+\Delta t) = \mathbb{M}(\Delta t)\cdot\mathbb{X}_0$$
$$= \mathbb{M}^{(p-1)}(\Delta t/p)\cdot\mathbb{X}_0$$

Compounded Push Operator:

- Uniform Field Push can be Subdivided
- Can be Written as Product of δt Substeps

$$
\begin{aligned}
\mathbb{X}(t+\Delta t) &= \mathbb{M}(\Delta t)\cdot\mathbb{X}_0 \\
&= \mathbb{M}^{(p-1)}(\Delta t/p)\cdot\mathbb{X}_0 \\
&= \prod_{k=0}^{p-1}\mathbb{M}^{[k]}(\delta t)\cdot\mathbb{X}_0
\end{aligned}
$$

Compounded Push Operator:

- Uniform Field Push can be Subdivided
- Can be Written as Product of δt Substeps
- Also True if $\mathbb{M}^{[k]}$ varies with t – Equivalent to Explicit Stepping with Smaller Δt

$$\begin{aligned}
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\end{aligned}$$

Compounded Push Operator:

- Uniform Field Push can be Subdivided
- Can be Written as Product of δt Substeps
- Also True if $\mathbb{M}^{[k]}$ varies with t – Equivalent to Explicit Stepping with Smaller Δt
- Estimator for $\mathbb{M}^{[k]}$ Reduces Field Evaluations, but not Push Multiplier Operations...

$$
\begin{aligned}
\mathbb{X}(t+\Delta t) &= \mathbb{M}(\Delta t)\cdot\mathbb{X}_0 \\
&= \mathbb{M}^{(p-1)}(\Delta t/p)\cdot\mathbb{X}_0 \\
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\end{aligned}
$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...

$$\widetilde{\mathbb{M}} = \prod_{k=0}^{p-1} \mathbb{M}^{[k]}$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...
- Can be Split into Mean and Deviation

$$\widetilde{\mathbb{M}} = \prod_{k=0}^{p-1} \mathbb{M}^{[k]} = \prod_{k=0}^{p-1} \left(\overline{\mathbb{M}} + \Delta\mathbb{M}^{[k]}\right)$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...
- Can be Split into Mean and Deviation
- The Operator is Linearized around $\overline{\mathbb{M}}$

$$
\begin{aligned}
\widetilde{\mathbb{M}} &= \prod_{k=0}^{p-1} \mathbb{M}^{[k]} \\
&= \prod_{k=0}^{p-1} \left(\overline{\mathbb{M}} + \Delta\mathbb{M}^{[k]}\right) \\
&= \prod_{k=0}^{p-1} \left(\mathbb{L}\Lambda\mathbb{R} + \Delta\mathbb{M}^{[k]}\right)
\end{aligned}
$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...
- Can be Split into Mean and Deviation
- The Operator is Linearized around $\overline{\mathbb{M}}$

$$\begin{aligned}\widetilde{\mathbb{M}} &= \prod_{k=0}^{p-1} \mathbb{M}^{[k]} \\ &= \prod_{k=0}^{p-1} \left(\overline{\mathbb{M}} + \Delta\mathbb{M}^{[k]}\right) \\ &= \mathbb{L}\left[\prod_{k=0}^{p-1}\left(\Lambda + \mathbb{R}\Delta\mathbb{M}^{[k]}\mathbb{L}\right)\right]\mathbb{R}\end{aligned}$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...
- Can be Split into Mean and Deviation
- The Operator is Linearized around $\overline{\mathbb{M}}$
- And Assuming $||\Lambda|| \gg ||\mathbb{R}\Delta\mathbb{M}^{[k]}\mathbb{L}||$

$$
\begin{aligned}
\widetilde{\mathbb{M}} &= \prod_{k=0}^{p-1} \mathbb{M}^{[k]} \\
&= \prod_{k=0}^{p-1} \left(\overline{\mathbb{M}} + \Delta\mathbb{M}^{[k]}\right) \\
&= \mathbb{L}\left[\prod_{k=0}^{p-1} \left(\Lambda + \mathbb{R}\Delta\mathbb{M}^{[k]}\mathbb{L}\right)\right]\mathbb{R} \\
&= \mathbb{L}\left[\Lambda^{(p-1)} + \sum_{k=0}^{p-2} \left(\Lambda^{(p-2)-k}\mathbb{R}\Delta\mathbb{M}^{[k]}\mathbb{L}\Lambda^{k}\right) + O(\Delta\mathbb{M}^2)\right]\mathbb{R}
\end{aligned}
$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...
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- Summations to Series Solution for Linear and Oscillatory Parts of $\Delta M \rightarrow$ Direct Eval of m_{ij}

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\widetilde{\mathbb{M}} &= \prod_{k=0}^{p-1} \mathbb{M}^{[k]} \\
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&= \mathbb{L}\left[\prod_{k=0}^{p-1} \left(\Lambda + \mathbb{R}\Delta\mathbb{M}^{[k]}\mathbb{L}\right)\right]\mathbb{R} \\
&= \mathbb{L}\left[\Lambda^{(p-1)} + \sum_{k=0}^{p-2}\left(\Lambda^{(p-2)-k}\mathbb{R}\Delta\mathbb{M}^{[k]}\mathbb{L}\Lambda^{k}\right) + O(\Delta\mathbb{M}^2)\right]\mathbb{R}
\end{aligned}$$

$$\begin{aligned}
m_{ij} &\approx \mathbb{L}\left[\lambda_i^{(p-1)} + \lambda_i^{(p-2)}\mathbb{Q}_{ij}\sum_{k=0}^{p-2}\left[f_Q(k)\lambda_{j\setminus i}^{k}\right]\right]\mathbb{R} \\
&\approx \mathbb{L}\left[\lambda_i^{(p-1)} + \lambda_i^{(p-2)}\mathbb{Q}_{ij}\begin{cases}\sum k\lambda^k, \\ \sum cos(\alpha k)\lambda^k, \\ \sum sin(\alpha k)\lambda^k\end{cases}\right]\mathbb{R}
\end{aligned}$$

Operation Reduction:

- Given the Gyro-Estimated Compounded Operator $\widetilde{\mathbb{M}}$...
- Can be Split into Mean and Deviation
- The Operator is Linearized around $\overline{\mathbb{M}}$
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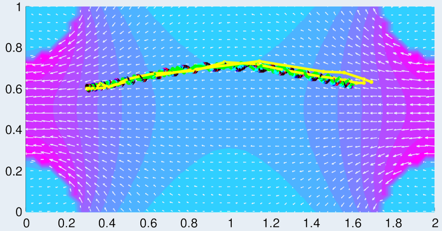


Magnetic Mirror Test

Elementary processes (electron-impact only)

- Collisional excitation/deexcitation

$$H(i) + e^- \leftrightarrow H(j) + e^-$$

- Collisional ionization/recombination

$$H(i) + e^- \leftrightarrow H^+ + 2e^-$$

- Bound-bound radiative transition

$$H(i) + h\nu \leftarrow H(j)$$

Rate Equation

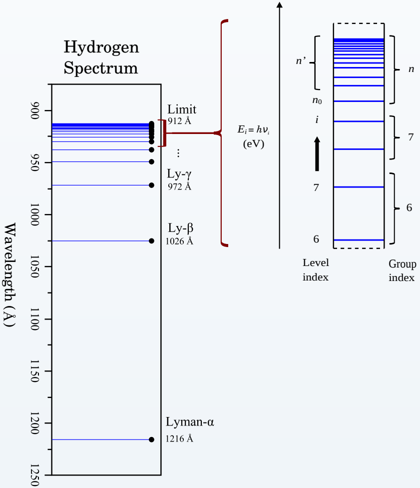
$$K_{ji}^{rad.} = A_{ji}, \quad K_{ji}^{coll.} = N_e \int_{E_{ij}}^{\infty} \sigma_{ij}(\varepsilon) v f(\varepsilon) d\varepsilon$$

$$\frac{dN_i}{dt} = \sum_{R \in \mathrm{Rxn}} \sum_{j \neq i} (K_{ij}^R N_j - K_{ji}^R N_i)$$

$$dN_i = \sum_{j \neq i} \tilde{\mathbf{K}}_{ij} N_j - \tilde{\mathbf{J}}_i \circ N_i$$

Implicit formulation

$$dN_j = \mathbb{A}_{ij}^{-1} \left[\sum_{j \neq i} \tilde{\mathbf{K}}_{ij} N_j - \tilde{\mathbf{J}}_i \circ N_i \right]$$

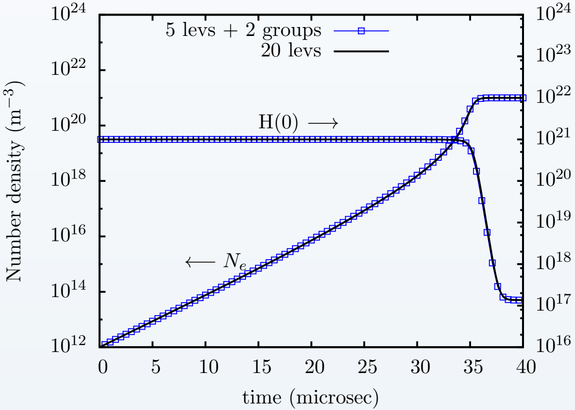


Hydrogen Spectrum
Wavelength (Å)
900
950
1000
1050
1100
1150
1200
1250
Limit
912 Å
Ly-γ
972 Å
Ly-β
1026 Å
Lyman-α
1216 Å
$E_i = h\nu_i$
(eV)
n'
n
n_0
i
7
6
7
6
Level index
Group index

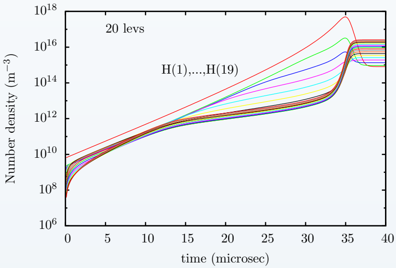
n,m: bin indices; i,j: level indices

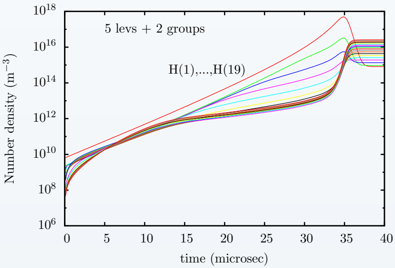
Model	Cons. vars.	Size	Lev. Pop.
Full CR	N_i	N_{level}	
Reduced CR (Uniform)	$\Sigma_n = \sum_{i \in n} N_i$	N_{group}	$N_{i \in n} = \frac{g_i \Sigma_n}{\sum_{j \in n} g_j}$
Reduced CR (Boltzmann)	N_{n_0} $\Sigma'_n = \sum_{i \in n'} N_i$	$2 \times N_{\text{group}}$	$N_{i \in n} = \frac{g_i N_{n_0} e^{-\Delta E_i / kT_n}}{g_{n_0}}$ or $N_{i \in n} = \frac{g_i \Sigma'_n e^{-\Delta E_i / kT_n}}{Q'_n}$

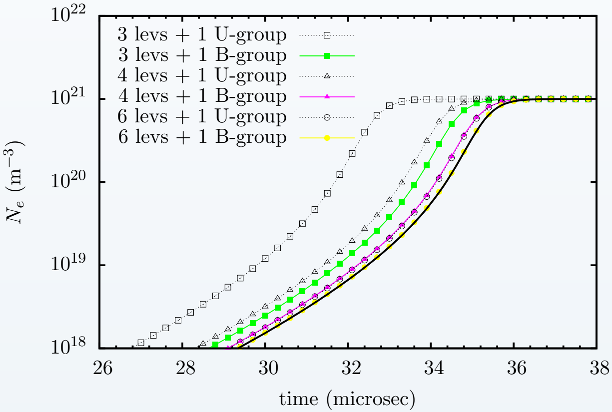
Comparison of ground state and electron number densities



Comparison of excited states number densities

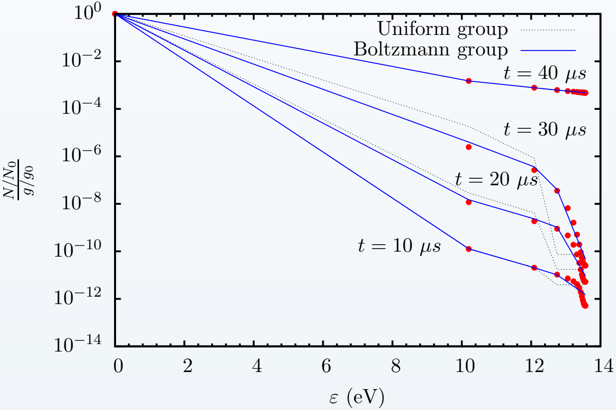






3 levs + 1 U-group
3 levs + 1 B-group
4 levs + 1 U-group
4 levs + 1 B-group
6 levs + 1 U-group
6 levs + 1 B-group
N_e (m^{-3})
10^{22}
10^{21}
10^{20}
10^{19}
10^{18}
26 28 30 32 34 36 38
time (microsec)

Uniform vs. Boltzmann



Numerous Previous Merge Methods:

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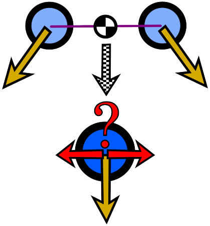
- 2:1 - Cannot Conserve Energy
  (Lapenta & Brackbill, JCP 1994)

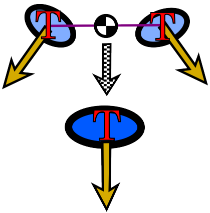


$$w_m = \sum w_i$$
$$\vec{v}_m = \sum w_i \vec{v}_i / w_m$$

$$w_m v_m^2 < \sum w_i v_i^2 \; !!!$$

Numerous Previous Merge Methods:

- 2:1 - Cannot Conserve Energy
  (Lapenta & Brackbill, JCP 1994)
- Complex Macro-particles with Internal Energy
  (Hewett, JCP 2003)



$$w_m = \sum w_i, \quad \vec{v}_m = \sum w_i \vec{v}_i / w_m$$

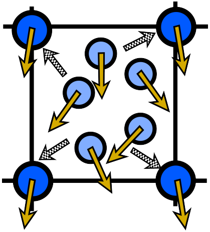
$$T_m^{(int)} = \left(\sum w_i T_i^{(int)} + \sum w_i v_i^2 - w_m v_m^2 \right) / w_m$$

$$w_m \left(v_m^2 + T_m^{(int)} \right) = \sum \left(w_i v_i^2 + w_i T_i^{(int)} \right) \checkmark$$

Particle Push with $T^{(int)}$?...
Split if $\left(T^{(int)}\right)^{1/2} \gg v_m$?...
In What Coord-System?...

Numerous Previous Merge Methods:

- 2:1 - Cannot Conserve Energy
  (Lapenta & Brackbill, JCP 1994)
- Complex Macro-particles with Internal Energy
  (Hewett, JCP 2003)
- Merge to Grid
  (Assous et al., JCP 2003, Welch et al., JCP 2007)



Conserve Arbitrary Moments to Grid

Not Explicitly Conserved Lost?
Entropy Generation?
Shape Functions?
Grid Dependence?

Numerous Previous Merge Methods:

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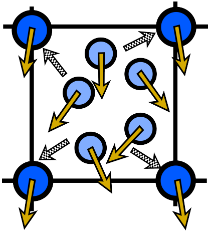
  (Lapenta & Brackbill, JCP 1994)
- Complex Macro-particles with Internal Energy
  (Hewett, JCP 2003)
- Merge to Grid
  (Assous et al., JCP 2003, Welch et al., JCP 2007)

All Introduce Significant Error and/or Complexity



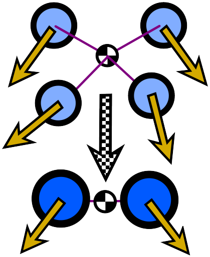
Conserve Arbitrary Moments to Grid

Not Explicitly Conserved Lost?
Entropy Generation?
Shape Functions?
Grid Dependence?

Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF

(AFOSR Review 2006)



$$w_m = \sum_i^{(n+2)} w_i$$
$$\bar{\vec{v}} = \left(\sum_i^{(n+2)} w_i \vec{v}_i\right) / w_m$$
$$\overline{V^2} = \left(\sum_i^{(n+2)} w_i \left(\vec{v}_i - \bar{\vec{v}}\right)^2\right) / w_m$$

$$w_{(a/b)} = w_m/2$$
$$\vec{v}_{(a/b)} = \bar{\vec{v}} \pm \hat{\mathcal{R}}\sqrt{\overline{V^2}}$$
$$\left(\text{Similarly: } \vec{x}_{(a/b)} = \bar{\vec{x}} \pm \hat{\mathcal{R}}\sqrt{\overline{X^2}}\right)$$

Conservative Merge

Merge to Pair $\rightarrow$ DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
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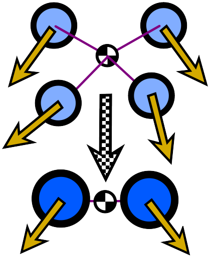
(AFOSR Review 2006)

Selection of Near Neighbors in VDF Limits Thermalization

($\approx$ Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)



$$w_m = \sum_i^{(n+2)} w_i$$

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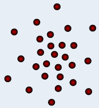
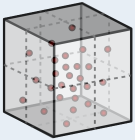
Phase-Space Decomposition

- Given a Set of Particles...



Phase-Space Decomposition

- Given a Set of Particles...
- Particles Binned in Octants



Phase-Space Decomposition

- Given a Set of Particles...
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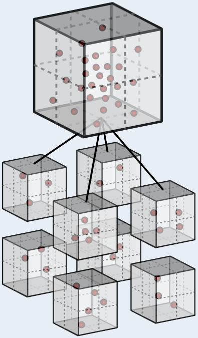
- Octants Recursively Sub-Divided



Phase-Space Decomposition

- Given a Set of Particles...
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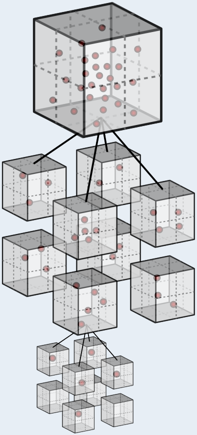

Octree Binning

Phase-Space Decomposition

- Given a Set of Particles...
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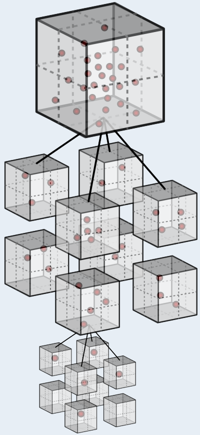
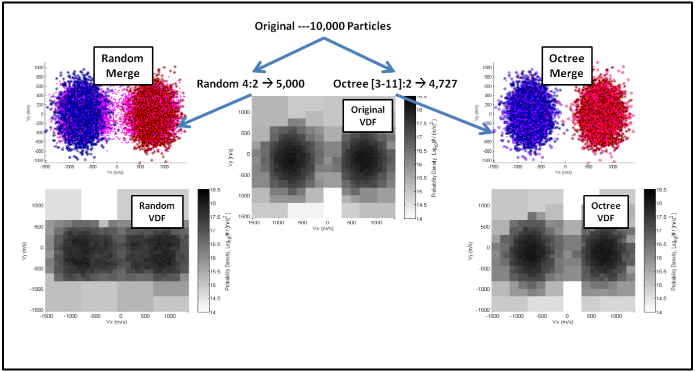
Restricts Phase-Space Diffusion to Within Local Bins



Comparison of Random vs. Octree Merge Partner Selection
(Note: Mass, Momentum, and Kinetic Energy Both Exactly Conserved)



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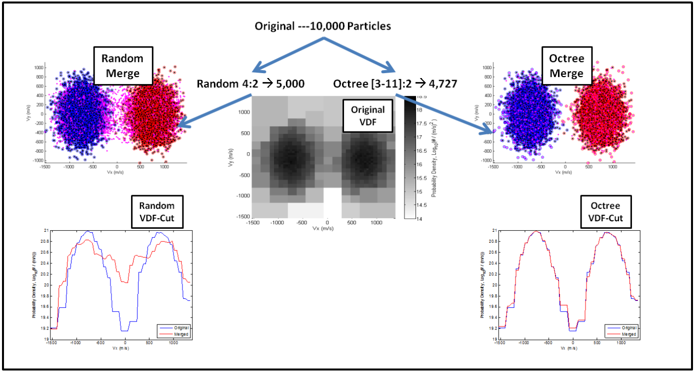
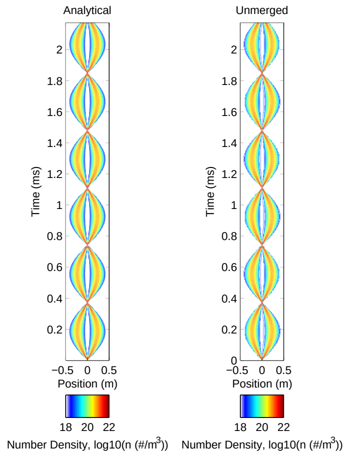


Collisionless Particles in Well

- 6000 Unmerged Particles
- Reproduces 3-4 Orders of Magnitude



Collisionless Particles in Well

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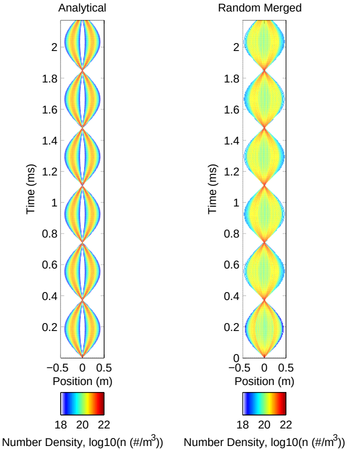
- Random Merge -> Thermalization
- 3000 First Point, 1500 First Cross
- Bi-Maxwellian Specifically Difficult



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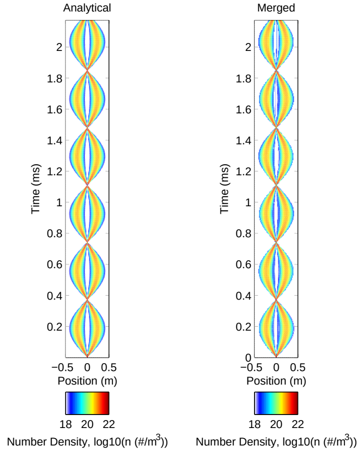

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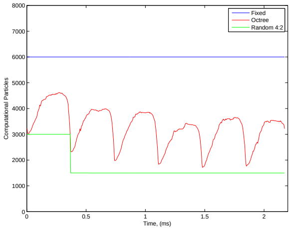

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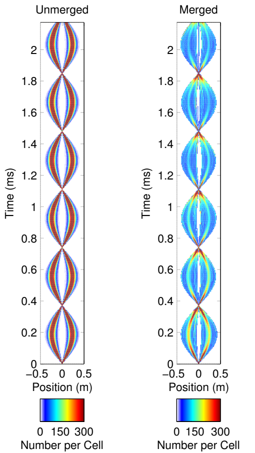
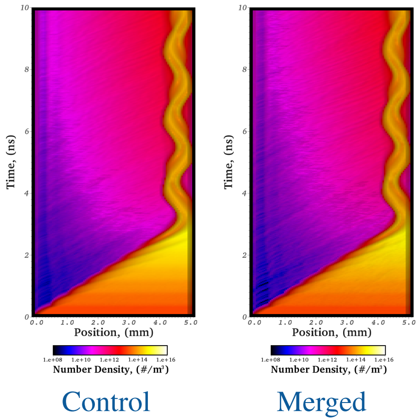
- Merge & Split Adapts Particle Count
- Computational Particles per Cell Vastly Different



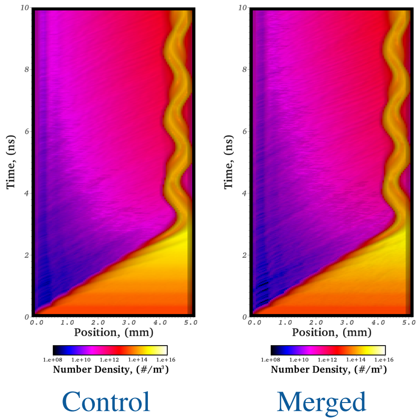
DC-Diode Test Case:

- Full 3D Electrostatic-PIC
- Averaged to 1D XT-Plot



DC-Diode Test Case:

- Full 3D Electrostatic-PIC
- Averaged to 1D XT-Plot
- 250V Cathode $\rightarrow$ Anode
- MCC-Ionization Collisions
- Secondary Emission at Cathode



DC-Breakdown

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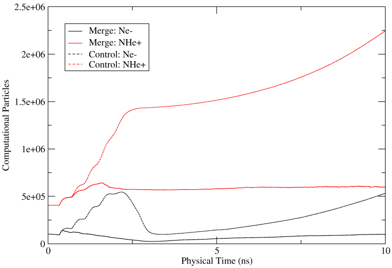
- Secondary Emission at Cathode
- Chain-Branching Needs Merge



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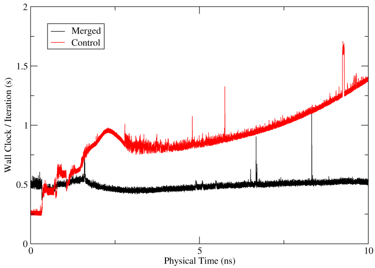
- Chain-Branching Needs Merge
- Merge Overhead Rapidly Negligible



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- Secondary Emission at Cathode
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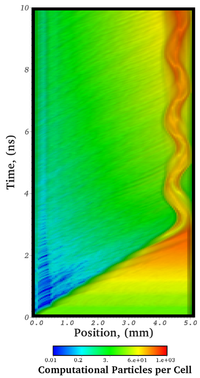
- Merge Overhead Rapidly Negligible
- Control: Parts/Cell $\propto$ Density



Control

Merged

DC-Breakdown

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- 250V Cathode $\rightarrow$ Anode
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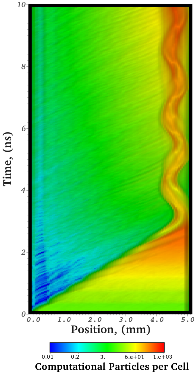
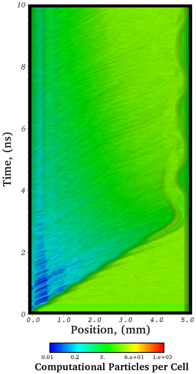
- Secondary Emission at Cathode
- Chain-Branching Needs Merge
- Merge Overhead Rapidly Negligible
- Control: Parts/Cell $\propto$ Density
- Merge: Parts/Cell Much Reduced



Control



Merged

DC-Diode Test Case:

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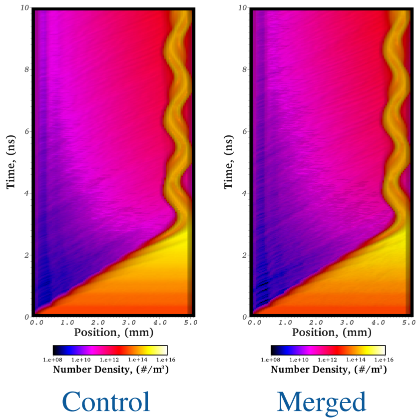
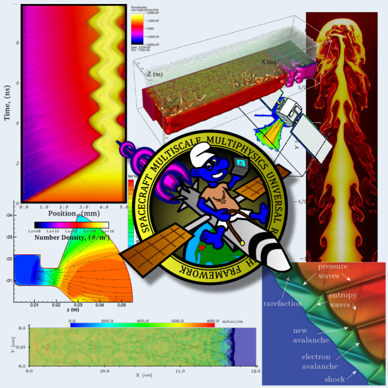
- 250V Cathode $\rightarrow$ Anode
- MCC-Ionization Collisions
- Secondary Emission at Cathode
- Chain-Branching Needs Merge
- Merge Overhead Rapidly Negligible
- Control: Parts/Cell $\propto$ Density
- Merge: Parts/Cell Much Reduced
- Despite Identical Densities



Integrate R&D w/ Production TODO:

- High-Order Fluid/MHD GPU Models
  (Le/Cole*/Bilyeu PhD Research)
- GPU Accelerated Chemical Kinetics / CR Ar-Ne-Xe-Molecular Models
  (Le/Cole*/Kapper* PhD Research)
- Phase-Space Reconstruction/Vlasov
  (Martin/Bilyeu/TBD)
- Implicit / Multiscale GPU-Accelerated PIC
  (Lederman/Gimelsheins/Martin/TBD)

*Note: Former Co-op Student Work to be Integrated into Framework



Thank You

Questions?